Quantum time correlation functions via noisy Monte Carlo and classical trajectories

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Abstract

Starting from a path integral representation, we show that, in its linearized form, Schofield's expression for the correlation function can be efficiently computed by averaging appropriate functions of coordinates and momenta over a set of classical trajectories [1]. The initial conditions for these trajectories are obtained from an exact representation of the quantum thermal density. To tame the effect of a phase factor, in this representation we use a cumulant expansion leading to a form for the density which can only be estimated numerically. To solve this difficulty, we adapt to our case advanced Monte Carlo methods for ``noisy" probability densities [2,3]. The efficiency of the algorithm is demonstrated by calculating the dynamic structure factor for a realistic model of liquid Neon [4]. We also show, by computing the gas phase infrared spectrum of a set of test molecules, that the method converges with a number of trajectories similar to that of other commonly adopted quasiclassical schemes that fail when applied to this calculation.

References

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